

1,6-Dichloro-1,6-dideoxyhex-2-ulofuranosyl 6-chloro-6-deoxyhexopyranoside  
40631-75-2 | DTXSID30315770

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 9.54e-01

Global applicability domain: Outside

Local applicability domain index: 2.30e-01

Confidence level: 6.75e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Tris(2-hydroxyethyl) isocyanurate</div> <div>Measured: 1.58</div> <div>Predicted: 1.61</div>	<div>Image not found</div> <div>Triisopropanolamine</div> <div>Measured: 5.75e-01</div> <div>Predicted: 7.42e-01</div>	<div>Image not found</div> <div>Malaoxon</div> <div>Measured: 1.12</div> <div>Predicted: 1.49</div>
<div>Image not found</div> <div>Hexamethylphosphoramide</div> <div>Measured: 5.01e-01</div> <div>Predicted: 7.23e-01</div>	<div>Image not found</div> <div>Triethyl phosphate</div> <div>Measured: 1.29</div> <div>Predicted: 1.38</div>	